ATOMIC AND MOLECULAR HYDROGEN IN THE THERMOSPHERE

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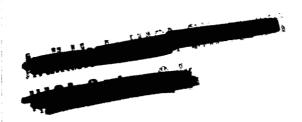
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ABSTRACT

Calculations are performed to determine the influence of a
layer of molecular hydrogen in the lower thermosphere, whose pre-
sence has been recently suggested by Bates and Nicolet, on the
escape rate and altitude distribution of atomic hydrogen in the
thermosphere. It is concluded that the presence of molecular
hydrogen has little affect on the distribution of atomic hydro-
gen.

1. Introduction

The abundance of hydrogen in the Earth's atmosphere in the region of and below 100 km has been considered recently by Bates and Nicolet[1]. They have noted that the reaction,

$$H + HO_2 \rightarrow H_2 + O_2 \tag{1}$$

may be an important source of hydrogen molecules in the mesosphere. Assuming that the hydrogen molecules are lost through the process,

$$H_2 + O \rightarrow OH + H \tag{2a}$$

the OH further reacting through the process,

$$OH + O \rightarrow O_2 + H \tag{2b}$$

they have concluded that a layer of hydrogen molecules is formed whose concentration is conceivably well above that of atomic hydrogen at the 100 km level. The molecular hydrogen would flow upwards through the thermosphere being converted to atomic hydrogen by processes (2a) and (2b). Bates and Nicolet[1] have noted that this mechanism would tend to increase the escape rate of atomic hydrogen.

In this paper the influence of hydrogen molecules on the escape rate and distribution of atomic hydrogen is investigated.

2. Diffusion Equations

The distributions of atomic and molecular hydrogen, assumed to be minor atmospheric constituents, are described by the equations,

$$\frac{dn_1}{dz} = -n_1 P_1 - \phi_1/Q_1 \tag{3}$$

$$\frac{dn_2}{dz} = -n_2 P_2 - \phi_2/Q_2 \tag{4}$$

$$\frac{d\phi_1}{dz} = 2\beta n_2 n(0) \tag{5}$$

$$\frac{d\phi_2}{dz} = -\beta n_2 n(0) \tag{6}$$

where,

$$P_i = [(1+\frac{m}{m_i}\Lambda_i)/H_i + (1+\alpha_i+\Lambda_i)\frac{d}{dz}\ln T]/(1+\Lambda_i) \tag{7}$$

and

$$Q_i = D_i(1+\Lambda_i) \tag{8}$$

The concentrations, fluxes, scale heights, molecular diffusion coefficients, ratios of the eddy to molecular diffusion coefficients, and thermal diffusion factors of the gases are denoted by n, ϕ, H, D, Λ and α respectively with identifying subscripts 1 for atomic hydrogen and 2 for molecular hydrogen. T is the gas temperature, β is the rate coefficient of process (2a), m is the mean mass per particle of the atmosphere, and $n(0)$ is the concentration of atomic oxygen. The rate coefficient, β, of

(2a) has been measured by Clyne and Thrush[2] over the temperature range 409°K to 733°K giving,

$$\beta = 6\times10^{-13} \, T^{1/2} \, \exp(-4450/T) \, cm^3 sec^{-1} \tag{9}$$

The molecular diffusion coefficients were taken to be,

$$D_1 = 2 \times 10^{18} \, T^{1/2}/N \tag{10}$$

and

$$D_2 = 1 \times 10^{18} \, T^{1/2}/N \tag{11}$$

where N is the total atmospheric gas concentration and the thermal diffusion factors were taken to be,

$$\alpha_1 = -0.25 \quad and \quad \alpha_2 = 0.33 \tag{12}$$

3. Model Atmospheres

In the region above 120 km the concentrations of the major constituents and the temperature were represented by the model introduced by Bates[3]. The temperature is given by

$$T(z) = T_\infty(1-e^{-\tau\xi}) \tag{13}$$

and the number density of component X by,

$$n(z/X) = n(120 \text{ km}/X) \left\{ \frac{1-a}{e^{\tau\xi}-a} \right\}^{1+\gamma} e^{\tau\xi} \tag{14}$$

where

$$a = [T_\infty - T(120 \text{ km})]/T_\infty \tag{15}$$

$$\tau = \left(\frac{dT}{dz}\right)_{z=120 \text{ km}} /[T_\infty - T(120 \text{ km})] \tag{16}$$

$$\gamma = [1-a]/\tau H(120 \text{ km}/X) \tag{17}$$

$H(120 \text{ km}/X)$ is the scale height of component X at the reference altitude of 120 km and ξ is the geopotential height above this reference level. The temperature at the escape level differs little from T_∞. It was assumed that,

$$n(120 \text{ km}/0) = 7.25 \times 10^{10} \text{ cm}^{-3} \tag{18}$$

$$n(120 \text{ km}/N_2) = 4.02 \times 10^{11} \text{ cm}^{-3} \tag{19}$$

$$n(120 \text{ km}/0_2) = 7.01 \times 10^{10} \text{ cm}^{-3} \tag{20}$$

$$T(120 \text{ km}) = 295°K, \left(\frac{dT}{dz}\right)_{z=120 \text{ km}} = 15°K/km \tag{21}$$

Below 120 km the temperature was assumed to take the form

$$T = T(120 \text{ km})[1+d\xi] \tag{22}$$

with

$$n(z/X) = n(120 \text{ km}/X)/[1+d\xi]^{1+b} \tag{23}$$

where

$$d = (\frac{dT}{dz})_{z=120 \text{ km}} / T(120 \text{ km}) \tag{24}$$

and

$$b = 1/dH(120 \text{ km}/X) \tag{25}$$

It was also assumed that,

$$(\frac{dT}{dz})_{z \leq 120 \text{ km}} = 4.25^\circ K/km \tag{26}$$

in this lower region. The values chosen for the atmospheric parameters are characteristic of the mean of the solar cycle[4]. The distribution of atomic oxygen is of some importance since, though reaction (2a) it is responsible for the destruction of molecular hydrogen. It is difficult to describe its distribution in the region below 120 km since this is controlled by the upwa diffusion (molecular and eddy) and dissociation of molecular oxygen. The work of Colegrove, Hanson and Johnson[5] appears to indicate that between 100 km and 120 km, atomic oxygen is best represented as following its own constant scale height, H(120 km/0), rather than a mixing scale height and this variation was adopted here.

Fig. 1 shows the lifetime of a hydrogen molecule defined by

$$\tau = 1/\beta n(0) \tag{27}$$

as a function of altitude for this model atmosphere for the cases of T_∞ of (13) equal to $1000^\circ K$ and $1750^\circ K$. It can be seen that the chemistry is of little importance below 120 km.

4.   Solution of the Diffusion Equations

Eqs. (5) and (6) imply that $\phi_1 + 2\phi_2$ is constant with altitude. At the escape level, taken to be at 500 km, ϕ_2 was set to zero so that

$$\phi_1 + 2\phi_2 = F \qquad (28)$$

where F is the escape flux of atomic hydrogen given approximately by,

$$F = 2.97 \times 10^7 \, n_1(500 \text{ km}) \, T(500 \text{ km})^{1/2} \quad \exp[-7010/T(500 \text{ km})] . \qquad (29)$$

Eqs. (3), (4) and (5) were numerically integrated downwards from the 500 km level to the 100 km level with,

$$n_1(500 \text{ km}) = 10^5; \quad \phi_1(500 \text{ km}) = F; \quad \phi_2(500 \text{ km}) = 0 \qquad (30)$$

Since the equations are linear the choice of $n_1(500 \text{ km})$ is arbitrary. Solutions were obtained for several values of $n_2(500 \text{ km})$ and for T_∞ of (13) equal to 750°K, 1000°K, 1250°K, 1500°K and 1750°K. The work of Colegrove et al.[5] indicates that the eddy diffusion coefficient may lie in the range $8 \times 10^5 \text{ cm}^2 \text{ sec}^{-1}$ to $8 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$. Since, at the 100 km level D_1 has a value of $3.4 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$ rising to $7.3 \times 10^7 \text{ cm}^2 \text{ sec}^{-1}$ at 120 km the inclusion of eddy diffusion is of interest. Calculations were therefore performed with the eddy diffusion coefficient, D_E, set equal to zero, $2 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$ and $4 \times 10^6 \text{ cm}^2 \text{ sec}^{-1}$ at all altitudes.

Equations (4) and (6) do not involve n_1 so that the solutions n_2 and ϕ_2 may be obtained independent of the n_1 distribution. Table 1 shows w_2 (100 km), the diffusion velocity of molecular hydrogen at the 100 km level as well as w_1 (100 km), the diffusion velocity of atomic hydrogen at the 100 km level in the absence of molecular hydrogen. The results are given for various values of the eddy diffusion coefficient, D_E, and the temperature, T_∞. The molecular diffusion coefficients appear to be large enough to prevent any significant dependence of the solutions on D_E. '

If both components followed a mixing distribution at low altitudes the appropriate diffusion velocities for w_1 (100 km) and w_2 (100 km) would be 4.9 cm sec^{-1} and 2.2 cm sec^{-1} respectively*. It can therefore be seen from the table that there is a departure from the mixing distribution although it is not very significant. Except at low temperatures, when the escape flux is small enough to cause the atomic hydrogen distribution to follow its own scale height to lower altitudes than at higher temperatures, the results are rather insensitive to T_∞ .

It is also possible to derive a relationship between n_1 and n_2 independent of the boundary conditions and hence deduce the effect of

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*These figures depend on the model atmosphere choosen and the values assigned to the diffusion coefficients D_1 and D_2. For example, Kocharts and Nicolet[6] obtain a value of 2.5 cm sec^{-1} for w_1 (100 km).

molecular hydrogen on the escape flux of atomic hydrogen. Let n_1, ϕ_1 and n_1^*, ϕ_1^*, be respectively solutions to the diffusion equations corresponding to the solutions n_2 and n_2^*. It can be shown that,

$$\frac{dG}{dz} - G(P_2 - \Gamma_1 + w_2/Q_2) = 2w_2/Q_1 \tag{31}$$

where

$$G = (n_1^* - n_1)/(n_2^* - n_2) \quad . \tag{32}$$

The boundary condition on G is that $G(500 \text{ km}) = 0$ since $n_1(500 \text{ km})$ and $n_1^*(500 \text{ km})$ were arbitrarily fixed at 10^5. G is thus independent of the distributions n_1, n_1^*, n_2, and n_2^*. Setting $n_2^* = 0$ at all altitudes, n_1^* becomes the atomic hydrogen distribution obtained when molecular hydrogen is absent, denoted by $n_1^{(0)}$. Thus (32) gives,

$$n_1(z) = n_1^{(0)}(z) + n_2(z)G(z) \quad . \tag{33}$$

Table 2 gives the values of G (100 km) obtained from the numerical solutions for the exospheric temperatures and eddy diffusion coefficients considered.

Measurements of the terrestrial absorption of Solar Lyman-α radiation indicate that n_1 (100 km)$\approx 10^7$ cm^{-3}. If the escape flux in the absence of molecular hydrogen is to be augmented by a factor f while still maintaining n_1 (100 km) $= 10^7$ cm^{-3} then it follows from (33) that,

$$n_2(100 \text{ km}) = (1-f)10^7/G(100 \text{ km}) \quad . \tag{34}$$

Bates and Nicolet[1] find the total upward flux of hydrogen atoms (both free and combined) from the lower atmosphere to be about 8×10^7 cm^{-2} sec^{-1} which must equal the escape flux. Table 2 shows the values of n_2 (100 km), calculated from (34), necessary to augment the escape flux in the absence of molecular hydrogen to this value. For example about $1.3_2 \times 10^7$ and $1.2_0 \times 10^7$ hydrogen molecules/cm^3 are required at 100 km for the cases of T = 1000°K and 1750°K respectively with the eddy diffusion coefficient $D_E = 4 \times 10^6$ cm^2 sec^{-1}. Figs. 2 and 3 show the atomic and molecular hydrogen distributions and fluxes for these two cases. The dashed curves show the distributions of atomic hydrogen in the absence of molecular hydrogen while still producing the same escape flux. It can be seen that the atomic hydrogen distribution is not seriously affected by the presence of molecular hydrogen. Fig. 1 indicates that the greatest amount of atomic hydrogen is produced in the region of 200 km which is above the region where the gradient in the atomic hydrogen distribution is greatest. It is therefore, not surprising that the presence of molecular hydrogen in significant quantities does not seriously distort the atomic hydrogen distribution.

5. Conclusions

It appears that, at the 100 km level, a concentration of molecular hydrogen comparable to the atomic hydrogen concentration is consistent with the estimated flux of hydrogen from the lower atmosphere. The altitude distribution of atomic hydrogen is not appreciably affected by the presence of the molecular species.

Acknowledgements

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CAPTIONS

Figure 1   Lifetime of a hydrogen molecule as a function of altitude as regards destruction through process (2a) of the text.

Figure 2   Distribution and fluxes of atomic and molecular hydrogen corresponding to an escape flux of atomic hydrogen of 8×10^7 cm^{-2} sec^{-1} for $T_\infty = 1000°K$. The dashed curve is the distribution that would be obtained in the absence of molecular hydrogen.

Figure 3   Distribution and fluxes of atomic and molecular hydrogen corresponding to an escape flux of atomic hydrogen of 8×10^7 cm^{-2} sec^{-1} for $T_\infty = 1750°K$. The dashed curve is the distribution that would be obtained in the absence of molecular hydrogen.

TABLE 1

T_∞ °K	w_1 (100 km) cm sec^{-1} D_E cm^2 sec^{-1}			w_2 (100 km) cm sec^{-1} D_I cm^2 sec^{-1}		
	0	2×10^6	4×10^6	0	2×10^6	4×10^6
750	3.44	3.07	2.79	1.86	1.77	1.72
1000	4.12	3.94	3.80	1.88	1.80	1.75
1250	4.19	4.05	3.93	1.88	1.80	1.76
1500	4.21	4.07	3.97	1.88	1.81	1.77
1750	4.22	4.08	3.98	1.89	1.81	1.77

TABLE 2

T_∞ °K	$-G(100\ km)$			$n_2(100\ km)$ (units $10^7\ cm^{-3}$)		
	$D_E\ cm^2\ sec^{-1}$			$D_E\ cm^2\ sec^{-1}$		
	0	2×10^6	4×10^6	0	2×10^6	4×10^6
750	0.861	0.835	0.822	1.54	1.92	2.27
1000	0.869	0.849	0.840	1.08	1.21	1.32
1250	0.873	0.856	0.849	1.04	1.14	1.23
1500	0.868	0.848	0.839	1.04	1.14	1.21
1750	0.868	0.848	0.840	1.03	1.13	1.20

1000° K

1750° K

T (SECS)

10

1

0.1

0.01

$\phi(H)$

$\phi(H_2)$

1750° K

$n(H)$

$n(H_2)$

FLUX (CM⁻² SEC⁻¹)

10^4 10^5 10^6 10^7 10^8

10^5 10^6 10^7 10^8